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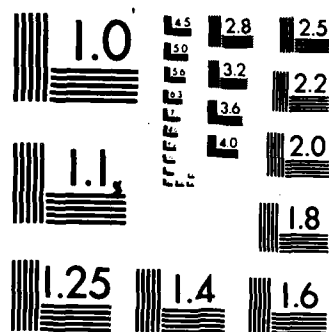
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Smoothing, Regularization and Ill-Posed  
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Estimation of Functions of Several Variables

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FINAL REPORT

Grace Wahba

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## 1. STATEMENT OF THE PROBLEMS STUDIED

Many problems were studied during the six year period of this research, 1 September 1977-30 September 1983 under the two titles:

Smoothing, Regularization, and Ill-Posed Inverse Problems

and

Robust and Convex Estimation of Functions of Several Variables and Associated Design Problems.

Sixteen Technical Reports and twenty papers and discussions appeared in the open literature.

Briefly, the problems studied fall in three classes:

(1) Problems density estimation, (2) Problems in experimental design, (3) Problems in the estimation of functions of one or several variables given noisy observations on functionals and various types of side and or prior information.

## SUMMARY OF THE MOST IMPORTANT RESULTS

Of the thirty six reports, papers and discussions that were written under the two subject contracts we believe that the two most important works are

G. Wahba, Improper priors, spline smoothing and the problem of guarding against model errors in regression. J. Roy. Stat. Soc. B, 40, 3, (1978)

and

M. Villalobos, Estimation of posterior probabilities using multivariate smoothing splines and generalized cross-validation. University of Wisconsin-Madison Statistics Department TR No. 725,(1983), thesis. The preparation for publication of a joint paper by Villalobos and Wahba is presently being supported by another agency.

The "Improper priors ..." paper popularized the cross validated smoothing spline and provided a general foundation for the development of the theory and practice of smooth nonparametric estimation of continuous functions from irregularly spaced, noisy data. The (univariate) cross validated smoothing spline discussed there is in general use, and code for it is widely available through the International Mathematical and Statistical Library as subroutine ICSSCV.

The "Estimation of posterior probabilities ..." report demonstrated that the cross validated bivariate thin plate spline with positivity and other linear inequality constraints is a feasible and effective tool for the smooth estimation of functions of two variables. We believe that the cross validated thin plate smoothing spline will come to have the same popularity as the univariate cross validated smoothing spline, and the feasibility and effectiveness of enforcing linear inequality constraints such as positivity will prove to be extremely useful.

3. TECHNICAL REPORTS PUBLISHED

1. G. Wahba, Data based optimal smoothing of orthogonal series density estimates, University of Wisconsin, Madison, Statistics Department, TR #509, January 1978.
2. G. Wahba, Improper priors, spline smoothing, and the problem of guarding against model errors in regression, University of Wisconsin, Madison, Statistics Department, TR #508, January 1978.
3. G. Wahba, Parameter estimation in linear dynamic systems. University of Wisconsin, Madison, Department of Statistics, TR #547, January 1979.
4. G. Wahba, How to smooth curves and surfaces with splines and cross-validation. University of Wisconsin-Madison, Department of Statistics, TR #555, March 1979.
5. H. Lucas, Choice of an optimal shape parameter when smoothing noisy data. University of Wisconsin, Madison, Department of Statistics TR #562, May 1979.
6. H. Lucas, Confidence regions for periodic functions. University of Wisconsin, Madison, Department of Statistics, TR #571, May 1979.
7. N. Dyn and G. Wahba, On the estimation of functions of several variables from aggregated data, Mathematics Research Center, University of Wisconsin, Technical Summary Report #1974, July 1979.
8. G. Wahba, Spline interpolation and smoothing on the sphere, University of Wisconsin, Madison, Department of Statistics TR #584, November 1979.
9. W.H. Wong, Expected information criterion for the smoothing parameter of density estimates: an elucidation of the modified likelihood, University of Wisconsin, Madison, Statistics Department TR 589, October 1979.
10. W. Knight, A comparison of some methods for flagging erroneous observations in certain types of meteorological data. University of Wisconsin, Madison, Statistics Department TR #610, May 1980.
11. G. Wahba, Bayesian confidence intervals for the cross validated smoothing spline, University of Wisconsin, Madison, Statistics Department TR #645,
12. G. Wahba, Numerical experiments with the thin plate histspline, University of Wisconsin, Madison, Statistics Department TR #638.
13. W.H. Wong, On constrained splines and their approximation, University of Chicago, Department of Statistics TR #127.
14. M. Villalobos and G. Wahba, Cross validated spline estimates for posterior probabilities in the classification problem, University of Wisconsin, Madison, Statistics Department TR #686, July 1982.



15. D. Nychka, G. Wahba, S. Goldfarb and T. Pugh, Cross validated spline methods for the estimation of three dimensional tumor size distributions from observations on two dimensional cross sections. University of Wisconsin, Madison, Statistics Department TR #711, June 1983.
16. M. Villalobos, Estimation of Posterior probabilities using multivariate smoothing splines and generalized cross validation. University of Wisconsin, Madison, Statistics Department TR #725, September 1983.

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1. G. Wahba and C. Micchelli, Lower Bounds for the Design Error in the Interpolation of Curves and Surfaces, (Abstract); The Institute of Mathematical Statistics Bulletin 8, 1, 1979, p. 48-49.
2. G. Wahba, Discussion to "Curve fitting and optimal design for prediction," by A. O'Hagan, J. Royal Statistical Society, Ser. B. 40, 1 (1978), p. 35-36.
3. G. Wahba, Discussion to "Density estimation, stochastic processes and prior information," by T. Leonard, J. Royal Statistical Society, Ser. B 40, 2 (1978), p. 140.
4. G. Wahba, Improper priors, spline smoothing and the problem of guarding against model errors in regression. J. Roy. Stat. Soc. B. 40, 3, 1978.
5. N. Dyn, G. Wahba and W.H. Wong, Invited discussion to "Smooth pychnophylactic interpolation". W. Tobler, J. Am. Stat. Soc., 74, 367 (1979), 530-535.
6. G. Wahba, How to smooth curves and surfaces with splines and cross validation. In "Proceedings of the 24th Conference on the Design of Experiments in Army Research Development and Testing", ARO Report 79-2, U.S. Army Research Office, Research Triangle Park, North Carolina.
7. H. Gamber, Choice of an optimal shape parameter when smoothing noisy data. Communications in Statistics, A8(14), 1425-1435 (1979).
8. H. Gamber, Confidence regions for periodic functions. Communications in Statistics, A8(14), 1437-1446 (1979).
9. G. Wahba, Parameter estimation in linear dynamic systems. IEEE Transactions on Automatic Control AC-25, No. 2, April 1980.
10. G. Wahba, Spline bases, regularization, and generalized cross validation for solving approximation problems with large quantities of noisy data. Proceedings of the International Conference on Approximation Theory in Honor of George Lorenz, Jan. 8-11, 1980, Austin Texas, Ward Cheney, ed., Academic Press (1980).
11. G. Wahba, Data-based optimal smoothing of orthogonal series density estimates, Ann. Statist. 9, 1 (1981).
12. G. Wahba, Spline interpolation and smoothing on the sphere. SIAM J. Scientific and Statistical Computing, 2, 1, 1981, 5-16.
13. N. Dyn and G. Wahba, On the estimation of functions of several variables from aggregated data, SIAM J. Math. Anal., 13, 1, (1982), 134-152.
14. G. Wahba, Numerical experiments with the thin plate histospline, Commun. Statist.-Theor. Meth. A10(24), (1981), 1475-2514.

15. F. O'Sullivan, Remote sensing of temperature profiles in the atmosphere. In Proceedings of the NASA Workshop on Density Estimation and Function Smoothing. L.F. Guseman, Jr., ed., Department of Mathematics, Texas A&M University, College Station, TX, 1982.
16. D. Nychka, Solving integral equations with noisy data: an application of smoothing splines in pathology. In proceedings of Interface XIV, July 6-7, 1982, Troy, N.Y., Karl Heiner, ed.
17. T.D. Pugh, J.H. King, H. Koen, D. Nychka, J. Chover, G. Wahba, Y. He, and S. Goldfarb, Reliable stereological methods for estimating the number of microscopic hepatocellular Foci from their transections. Cancer Research 43, 1261-1268, March 1983.
18. M. Villalobos and G. Wahba, Multivariate thin plate spline estimates for posterior probabilities in the classification problem. Commun. in Statis., 12, 1449-1480, 1983.
19. T. Pugh, J. King, H. Koen, Y. He., D. Nychka, S. Vesselinovitch, J. Chover, G. Wahba and S. Goldfarb, An improved method for quantitating neoplastic foci during hepatocarcinogenesis. Proc. Am. Assoc. Cancer Res., 23: 105, 1982.
20. D. Nychka, T.D. Pugh, J.H. King, H. Koen, G. Wahba, J. Chover and S. Goldfarb, Computer simulation studies of mathematical methods for estimating the number of hepatocellular foci in tissue sections. To appear, Cancer Research.

5. LIST OF PARTICIPATING SCIENTIFIC PERSONNEL AND DEGREES AWARDED

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Finbarr O'Sullivan	Ph. D.
Andrew Kirsch	M. S.
W.-H. Wong	Ph. D.
James Wendelberger	Ph. D.
Heather Lucas Gamber	Ph. D.
Anne Shoemaker	M. S.

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Sixteen technical reports and twenty other papers and discussions prepared by Professor Grace Wahba and associates, partially or wholly supported by the USARO, are listed. Major results include the development of univariate and multivariate cross validated splines for the smooth estimation of functions of one and several variables, and the extension of spline theory to encompass indirect measurements and linear inequality constraints, to provide confidence intervals, and to provide efficient numerical methods. Applications in Meteorology and Cancer Research were demonstrated.		

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